

Practical Calculation Scheme for Generalized Seniority

L. Y. Jia^{1,2,*}

¹*Department of Physics, University of Shanghai for Science and Technology, Shanghai 200093, P. R. China*

²*Department of Physics, Hebei Normal University, Shijiazhuang, Hebei 050024, P. R. China*

(Dated: February 11, 2014)

We propose a scheme or procedure for doing practical calculations with generalized seniority. It reduces the total computing time by calculating and storing in advance a set of intermediate quantities, taking advantage of the memory capability of modern computers. The requirements and performance of the algorithm are analyzed in detail.

PACS numbers: 21.60.Ev, 21.10.Re,

Keywords:

I. INTRODUCTION

Generalized seniority has long been introduced [1–4] in nuclear physics as an effective truncation scheme for the nuclear shell model. In the presence of strong pairing correlations, the nucleons form pairs and the ground state of an even-even nucleus is usually well approximated by a pair condensate. For the low-lying states the number of broken pairs should be small because naively breaking each pair costs about 2 MeV in energy (pairing energy). Consequently, generalized seniority S is introduced as the number of particles not participating in the coherent pair condensate (unpaired particles), and it is usually a good approximation to truncate the full many-body space to the one consisting of the states with low seniority.

In the literature there are many ways to calculate the matrix elements of operators between states with fixed seniority. Explicit expressions in various forms have been derived for cases of the lowest seniorities [4–12] and applied to realistic nuclei [13–16], but for higher seniority these expressions rapidly become cumbersome and have only formal meanings. Recently recursive relations for the matrix elements were derived [17] using the angular-momentum coupled version of the Wick’s theorem [20, 21], however in realistic calculations these relations may become very time consuming and up to now the method has only been carried out for $S \leq 2$ (one broken pair for each species of nucleons) [18, 19].

Computers have enjoyed rapid growth recently, in both computing speed and data storage capacity. Nowadays it is common to have several gigabyte memory in one’s laptop, and several terabyte memory at a workstation. The aim of this work is to propose an algorithm or procedure of generalized seniority that reduces the total time costs by utilizing the huge memories. The matrix elements of operators between seniority states are calculated in two steps. We first compute and store in memory the “density matrix” on the pair condensate that characterizes the properties of the latter. Then the matrix elements

of operators are expressed in terms of the “density matrix” through simple relations. In Sec. II we introduce the “density matrix” and derive recursive relations for its calculation. The simple routine is given to express the matrix elements of operators between seniority states in terms of the “density matrix”. Section III is devoted to the seniority truncation of the shell model. We formulate the procedure explicitly, the requirements (speed and memory) and performance of the algorithm are analyzed in detail. Finally in Sec. IV we summarize the work.

II. MATRIX ELEMENTS ON THE PAIR CONDENSATE

In this section we consider the matrix elements of operators on the pair condensate. The pair-creation operator

$$P_1^\dagger = a_1^\dagger a_{\bar{1}}^\dagger \quad (1)$$

creates a pair of particles on the single-particle level $|1\rangle$ and its time-reversed partner $|\bar{1}\rangle$ ($|\bar{1}\rangle = -|1\rangle$). The coherent pair-creation operator

$$P^\dagger = \sum_{\alpha} v_{\alpha} P_{\alpha}^\dagger \quad (2)$$

creates a pair of particles coherently distributed with structure coefficients v_{α} over the entire single-particle space. In Eq. (2) the summation index α is the “pair index” that runs over only half of the single-particle space ($P_1 = P_{\bar{1}}$). In the presence of pairing correlations, the seniority zero state of the $2N$ -particle system is

$$|\phi_N\rangle = \frac{1}{\sqrt{\chi_N}} (P^\dagger)^N |0\rangle, \quad (3)$$

where

$$\chi_N = \langle 0 | P^N (P^\dagger)^N | 0 \rangle \quad (4)$$

is the normalization factor. In addition, we introduce the pair-transfer amplitudes

$$t_{\alpha_1 \alpha_2 \dots \alpha_p; \beta_1 \beta_2 \dots \beta_q}^M = \langle 0 | P^{M-p} P_{\alpha_1} P_{\alpha_2} \dots P_{\alpha_p} P_{\beta_1}^\dagger P_{\beta_2}^\dagger \dots P_{\beta_q}^\dagger (P^\dagger)^{M-q} | 0 \rangle, \quad (5)$$

*Electronic address: liyuan.jia@usst.edu.cn

where *by definition all the “pair indices”* $\alpha_1, \dots, \alpha_p, \beta_1, \dots, \beta_q$ are different. The real number $t_{\alpha_1\alpha_2\dots\alpha_p;\beta_1\beta_2\dots\beta_q}^M$ is symmetric under permutations within α indices or β indices; and $t_{\alpha_1\alpha_2\dots\alpha_p;\beta_1\beta_2\dots\beta_q}^M = t_{\beta_1\beta_2\dots\beta_q;\alpha_1\alpha_2\dots\alpha_p}^M$. The normalization χ_N defined in Eq. (4) is the special case of Eq. (5) when all the α and β indices are missing: $\chi_N = t_N^N$.

Recursive relations for t (5) exist because operators P_1^\dagger (1), $P_1 = (P_1^\dagger)^\dagger = a_1^\dagger a_1$, and $\hat{N}_1 = \frac{1}{2}(a_1^\dagger a_1 + a_1 a_1^\dagger)$ form a closed algebra:

$$[P_1, P_1^\dagger] = 1 - 2\hat{N}_1, \quad [\hat{N}_1, P_1^\dagger] = P_1^\dagger. \quad (6)$$

From Eqs. (2) and (6) it is easy to derive the identity

$$P_\alpha(P^\dagger)^N|0\rangle = v_\alpha N(P^\dagger)^{N-1}|0\rangle - (v_\alpha)^2 N(N-1)P_\alpha^\dagger(P^\dagger)^{N-2}|0\rangle,$$

and consequently the recursive relations for the quantity t (5),

$$t_{\alpha_1\alpha_2\dots\alpha_p;\beta_1\dots\beta_q}^M = v_{\alpha_p}(M-q)t_{\alpha_1\alpha_2\dots\alpha_{p-1};\beta_1\dots\beta_q}^{M-1} - (v_{\alpha_p})^2(M-q)(M-q-1)t_{\alpha_1\alpha_2\dots\alpha_{p-1};\alpha_p\beta_1\dots\beta_q}^{M-1}. \quad (7)$$

The simplest case of Eq. (7) gives the recursive relation for the one-pair transfer amplitudes when there is only

one α subscript on t ,

$$t_{\alpha;}^M = \langle 0|P^{M-1}P_\alpha(P^\dagger)^M|0\rangle = v_\alpha M\chi_{M-1} - (v_\alpha)^2 M(M-1)t_{\alpha;}^{M-1}, \quad (8)$$

which is Eq. (22) in Ref. [22]. The normalization (4) is calculated as

$$\chi_N = \sum_{\alpha} v_{\alpha} t_{\alpha;}^N. \quad (9)$$

The most general operator is written schematically as a product of single-particle annihilation and creation operators, its matrix element on the pair condensate (3) is

$$\langle 0|P^M a_{i_1} a_{i_2} \dots a_{i_p} a_{j_1}^\dagger a_{j_2}^\dagger \dots a_{j_q}^\dagger (P^\dagger)^N |0\rangle, \quad (10)$$

where $i_1, \dots, i_p, j_1, \dots, j_q$ are single-particle indices that take values from the entire single-particle space (both $|1\rangle$ and $|\bar{1}\rangle$ are allowed), and $2M + p = 2N + q$ guarantees particle-number conservation. In order for the matrix element (10) to be nonzero, the indices i_1, i_2, \dots, i_p and j_1, j_2, \dots, j_q must differ in time-reversed pairs, because in $(P^\dagger)^N|0\rangle$ and $\langle 0|P^M$ the single-particle levels are occupied in time-reversed pairs. An example is

$$\begin{aligned} & \langle 0|P^{N-1} a_{\bar{1}} a_1 a_{\bar{2}} a_2 a_{\bar{3}} a_3 a_{\bar{4}} a_4 a_{\bar{5}} a_5 a_{\bar{6}} a_6 a_{\bar{7}} a_7 a_6^\dagger a_5^\dagger a_4^\dagger a_3^\dagger a_2^\dagger a_1^\dagger a_8^\dagger a_8^\dagger (P^\dagger)^N |0\rangle \\ &= \langle 0|P_1 P_1^\dagger |0\rangle \langle 0|P_3 P_3^\dagger |0\rangle \langle 0|a_5 a_6 a_7 a_7^\dagger a_6^\dagger a_5^\dagger |0\rangle \langle 0|^{[1,3,5,6,7]} P^{N-1} P_2 P_4 P_8^\dagger (P^\dagger)^N |0|^{[1,3,5,6,7]} \rangle = t_{2,4;8}^{N+1[1,3,5,6,7]}, \end{aligned} \quad (11)$$

where $|0|^{[1,3,5,6,7]}$ represents a subspace of the original single-particle space, by removing the single-particle levels $1, \bar{1}, 3, \bar{3}, 5, \bar{5}, 6, \bar{6}, 7, \bar{7}$ from the latter. This is the Pauli blocking effect; because operators P_1^\dagger , P_3^\dagger , and $a_7^\dagger a_6^\dagger a_5^\dagger$ (P_1 , P_3 , and $a_5 a_6 a_7$) could be moved to the rightmost (leftmost) side and their effects were simply blocking the corresponding pairs of single-particle levels. Similarly, $t_{2,4;8}^{N+1[1,3,5,6,7]}$ is defined as the pair-transfer amplitude in this restricted subspace. A formal analytical expression could be written down involving complicated Kronecker delta functions, but here we are content with the programmable routine described in Eq. (11).

The matrix element of an arbitrary operator O between states with fixed seniority could be written in the form (10): the product $a_{i_1} \dots a_{i_p} a_{j_1}^\dagger \dots a_{j_q}^\dagger$ consists of the operator O and the unpaired particles. From Eq. (11) we see that the matrix element of the form (10) boils down to the pair-transfer amplitudes t introduced in Eq. (5), *calculated in the original single-particle space and its subspaces*. These t 's play the role of “density matrix” for the pair condensate. They are the intermediate quan-

tities that appear repeatedly in the calculation and we would like to compute and store in advance to reduce the total time costs. In the next section we consider whether this is possible for realistic calculations within modern computers.

III. SENIORITY TRUNCATION OF SHELL MODEL

For simplicity we consider semi-magic even-even nuclei that have only one kind of active nucleons. The matrix elements of a two-body Hamiltonian between states with fixed seniority $2(\nu - \mu)$ and 2ν are schematically written as

$$\langle 0|P^{N+\mu} \underbrace{aa\dots a}_{2(\nu-\mu)} \underbrace{(aaa^\dagger a^\dagger)}_H \underbrace{a^\dagger a^\dagger \dots a^\dagger}_{2\nu} (P^\dagger)^N |0\rangle, \quad (12)$$

where $0 \leq \mu \leq \nu$. Following the procedure in Eq. (11) it boils down to the expression

$$t_{\alpha_1, \alpha_2, \dots, \alpha_{p-\mu}; \beta_1, \beta_2, \dots, \beta_p}^{[\gamma_1, \gamma_2, \dots, \gamma_r]}, \quad (13)$$

where in the scripts the number of α 's, β 's, and γ 's satisfy

$$p + \frac{r}{2} \leq \nu + 1 \leq p + r, \quad p \geq \mu. \quad (14)$$

Below we compute the number of different t 's at given μ , p , and r .

In the case of the spherical shell model with rotational symmetry, the single-particle space is generally written as $\{j_1, j_2, \dots, j_D\}$, each level j_i has degeneracy $2\Omega_i = 2j_i + 1$. The quantity t (13) is independent of the magnetic quantum number m : $t_{\dots, j_m, \dots}^{[\dots]} = t_{\dots, j_{m'}, \dots}^{[\dots]}$ for arbitrary m and m' ; similarly in the β and γ indices. Hence in this case we could write the quantity t (13) in “occupation representation” as

$$t_{n_1^\alpha, n_2^\alpha, \dots, n_D^\alpha; n_1^\beta, n_2^\beta, \dots, n_D^\beta; n_1^\gamma, n_2^\gamma, \dots, n_D^\gamma} \quad (15)$$

where n_i^α is the number of j_i 's (with arbitrary magnetic quantum number m_i) present in the series $\alpha_1, \alpha_2, \dots, \alpha_p$; similarly for n_i^β and n_i^γ . The following relations hold:

$$\sum_i n_i^\alpha = p - \mu, \quad \sum_i n_i^\beta = p, \quad \sum_i n_i^\gamma = r, \quad (16)$$

$$0 \leq n_i^\alpha + n_i^\beta + n_i^\gamma \leq \Omega_i, \quad 0 \leq n_i^\alpha, n_i^\beta, n_i^\gamma \leq \Omega_i. \quad (17)$$

We count the number of solutions $(n_i^\alpha, n_i^\beta, n_i^\gamma)$ of Eqs. (16) and (17) to get the number of different t 's at given μ , p , and r . In practice, the number of non-negative integer solutions satisfying Eq. (16) is $C_{r+D-1}^{D-1} C_{p+D-1}^{D-1} C_{p-\mu+D-1}^{D-1}$, from which we remove those violating Eq. (17).

In practical calculations we usually truncate the many-body space up to a maximum seniority $S = 2s$, thus the allowed values of the quartet (ν, μ, p, r) satisfy

$$0 \leq \nu \leq s, \quad 0 \leq \mu \leq \nu, \quad \mu \leq p \leq \nu + 1, \\ \nu + 1 - p \leq r \leq 2(\nu + 1 - p).$$

For each allowed triplet (μ, p, r) , we count the number of different t 's (13) based on Eqs. (16) and (17). Then we sum the results for all possible triplets (μ, p, r) to get the total number of t 's needed for a calculation truncated at seniority $S = 2s$. In Table I we list the numbers for realistic nuclear single-particle spaces. We see that it is indeed possible to store the intermediate quantities t (13) within the memory of modern computers, which have several gigabytes in a laptop and several terabytes at a workstation.

In summary, the procedure of doing a realistic calculation for even-even nuclei truncated at generalized seniority $S = 2s$ is: 1. Calculate the structure v_α (2) of the pair forming the condensate (3), for protons and neutrons separately. 2. Compute all the intermediate quantities t (13) based on the recursive relations (7), and store the results in memory. 3. Construct the many-body space consisting of basis states with fixed seniority up to S , additional truncation may be introduced to further reduce

the dimension. 4. Calculate the overlaps of the basis and the matrices of operators (e.g. the Hamiltonian) in a way similar to that of Eq. (11). 5. Diagonalize the sparse Hamiltonian matrix and calculate other observables.

A few comments are necessary. In step 1, the pair structure v_α (2) could be determined by the conventional way of minimizing energy, or by the recent method [22] based on the generalized density matrix that is much quicker in large model spaces [23]. The time cost of step 2 is not a problem at all, because computing each t (13) needs only a few multiplication operations according to Eq. (7), and the process is fully parallelable.

Step 4 is very similar to that of the “m-scheme” shell model but with two major differences. First, in the shell model a matrix element vanishes unless the operator series $aa\dots a$ from the left vector is the same (in one-to-one correspondence) as the series $a^\dagger a^\dagger \dots a^\dagger$ from the right vector, but here they could differ in time-reversed pairs. Thus the Hamiltonian matrix is less sparse compared with that of the shell model. Second, the value of the shell model matrix element is simply 1 (possibly with a phase “-1”), but here the matrix element boils down to a specific t that we should look up (for example by binary search) in the memory. This process is also parallelable and the time cost should not be a problem.

Even with the seniority truncation the many-body dimension becomes very large in big single-particle spaces at high seniority. The limiting factor in this situation should be the incapability of diagonalizing the huge Hamiltonian matrix, as was the case with the shell model. Thus in step 3 additional truncations beyond the seniority truncation could be introduced to further reduce the dimension of the many-body space. For example, in a two-major-shell calculation we could make the popular restriction that there was a maximum number c of *unpaired particles* that were allowed to be excited to the upper major shell. Please note that the actual number of particles on the upper shell could well exceed the number c , because the pairing condensate also has components in the upper shell (excitations due to pairing interaction). Another popular truncation was to use the collective pairs with certain multiplicity [11, 24–26] if the corresponding multipole-multipole interaction in the Hamiltonian was believed to be significant. Usually for the low-lying states the D pair (quadrupole pair with angular momentum two) is the most important one.

IV. SUMMARY

In conclusion, we propose a scheme for doing practical calculations with generalized seniority. The method utilizes the huge memory capabilities of modern computers by calculating and storing a set of intermediate quantities to reduce the total computing time costs. The requirements (memory and speed) and performance of the algorithm are analyzed in detail.

The limiting factor of the method is still the dimen-

sion of the many-body space. Even with the seniority truncation, in large single-particle spaces the many-body space may still become intractably huge at relatively high seniority. Thus additional truncations or restrictions on the unpaired particles may be necessary. Convergence should be reached for a specific observable with respect to the cutoffs of the truncations should the seniority results accurately reproduce the shell model results.

The current scheme of seniority calculations is similar in programming to that of the shell model. Thus it should be relatively easy to modify the existing well-

developed “m-scheme” shell model codes to get a good seniority code. Mature techniques used there could be adopted.

Support is acknowledged from the startup funding for new faculty member in University of Shanghai for Science and Technology. Part of the calculations is done at the High Performance Computing Center of Michigan State University.

-
- [1] I. Talmi, Nucl. Phys. **A172**, 1 (1971).
 - [2] S. Shlomo, I. Talmi, Nucl. Phys. **A198**, 81 (1972).
 - [3] K. Allaart, E. Boeker, G. Bonsignori, M. Savoia, Y.K. Gambhir, Phys. Rep. **169**, 209 (1988).
 - [4] Y.K. Gambhir, A. Rimini, T. Weber, Phys. Rev. **188**, 1573 (1969).
 - [5] Y.K. Gambhir, A. Rimini, T. Weber, Phys. Rev. C **3**, 1965 (1971).
 - [6] G. Bonsignori, M. Savoia, Nuovo Cimento A **44**, 121 (1978).
 - [7] S. Pittel, P.D. Duval, B.R. Barrett, Ann. Phys. (N.Y.) **144**, 168 (1982).
 - [8] O. Scholten and S. Pittel, Phys. Lett. **B120**, 9 (1983).
 - [9] A. Frank, P. Van Isacker, Phys. Rev. C **26**, 1661 (1982).
 - [10] P. Van Isacker, S. Pittel, A. Frank, P.D. Duval, Nucl. Phys. **A451**, 202 (1986).
 - [11] F. Iachello, A. Arima, The Interacting Boson Model, Cambridge University Press, Cambridge, 1987.
 - [12] T. Mizusaki, T. Ostuka, Prog. Theor. Phys. Suppl. **125**, 97 (1996).
 - [13] O. Scholten, H. Kruse, Phys. Lett. **B125**, 113 (1983).
 - [14] G. Bonsignori, M. Savoia, K. Allaart, A. van Egmond and G. te Velde, Nucl. Phys. **A432**, 389, (1985).
 - [15] J. Engel, P. Vogel, X. Ji, S. Pittel, Phys. Lett. **B225**, 5 (1989).
 - [16] O. Monnoye, S. Pittel, J. Engel, J.R. Bennett, P. Van Isacker, Phys. Rev. C **65**, 044322 (2002).
 - [17] F.Q. Luo, M.A. Caprio, Nucl. Phys. **A849**, 35 (2011).
 - [18] M. A. Caprio, F. Q. Luo, K. Cai, V. Hellemans, and Ch. Constantinou, Phys. Rev. C **85**, 034324 (2012).
 - [19] M. A. Caprio, F. Q. Luo, K. Cai, Ch. Constantinou, and V. Hellemans, J. Phys. G: Nucl. Part. Phys. **39**, 105108 (2012).
 - [20] J. Q. Chen, B. Q. Chen, A. Klein, Nucl. Phys. **A554**, 61 (1993).
 - [21] J. Q. Chen, Nucl. Phys. **A562**, 218 (1993).
 - [22] L. Y. Jia, Phys. Rev. C **88**, 044303 (2013).
 - [23] L. Y. Jia, Phys. Rev. C **88**, 064321 (2013).
 - [24] J. Q. Chen, Nucl. Phys. **A626**, 686 (1997).
 - [25] Y. M. Zhao, N. Yoshinaga, S. Yamaji, J. Q. Chen, and A. Arima, Phys. Rev. C **62**, 014304 (2000).
 - [26] N. Yoshinaga, and K. Higashiyama, Phys. Rev. C **69**, 054309 (2004).

TABLE I: Number of different t 's (13) needed for calculations truncated at generalized seniority $S = 2s$ in realistic single-particle spaces. The row labels represent single-particle spaces taken between two magic numbers; for example, “8 \sim 50” represents the space $\{0d_{\frac{5}{2}}, 0d_{\frac{3}{2}}, 1s_{\frac{1}{2}}, 0f_{\frac{7}{2}}, 0f_{\frac{5}{2}}, 1p_{\frac{3}{2}}, 1p_{\frac{1}{2}}, 0g_{\frac{9}{2}}\}$. For the suffix of numbers we have $1G = \chi M = \chi^2 k = \chi^3$, with $\chi = 1024 = 2^{10}$, following the convention in computers.

	$s = 1$	$s = 2$	$s = 3$	$s = 4$	$s = 5$	$s = 6$
20 \sim 50	846	7.42k	39.2k	135k	317k	537k
50 \sim 82	846	7.42k	39.5k	140k	351k	652k
82 \sim 126	1.63k	20.8k	161k	848k	3.18M	9.29M
8 \sim 50	4.28k	79.9k	845k	5.54M	25.2M	81.4M
20 \sim 82	10.2k	302k	5.10M	58.1M	468M	2.73G
50 \sim 126	14.7k	527k	10.9M	152M	1.48G	11.2G
8 \sim 82	26.9k	1.23M	32.9M	571M	6.76G	60.2G
28 \sim 126	47.1k	2.88M	104M	2.42G	40.8G	512G
0 \sim 126	201k	24.6M	1.70G	77.7G	—	—